List of Contents
and
Author Index
for
Computers and Chemistry

Volume 22

Computers & Chemistry

Chemistry • Biochemistry • Molecular Biology

editor

James Crabbe

Professor of Biochemistry, University of Reading, Wolfson Laboratory, AMS Building, Whiteknights, P.O. Box 228, Reading RG6 2AJ, U.K.

consulting editor

David Edelson

1107 Kenilworth Road, Tallahassee, FL 32312-3854, U.S.A.

editorial board

Dr P. H. Andersen
Novo Nordisk A/S
CNS Division
Novo Alle, DK-2880 Bagsvaerd
DENMARK

Dr Jan Andzelm
BIOSYM/Molecular Simulations Inc.
9685 Seranton Road, San Diego
CA 92121-3752, U.S.A.

Professor A. M. Bond
Department of Chemistry
Monash University, Clayton, Vic. 3169
AUSTRALIA

Dr J-M. Claverie
Laboratoire "Information Gènètique & Structurale"
IBSM-CNRS 31 Chemin Joseph Alguier
F-13402 Marseille Cedex 20
FRANCE

Dr J. Fickett
SmithKline Beecham Pharmaceuticals
Mail Code UW 2230
709 Swedeland Road, King of Prussia
PA 19406, U.S.A.

Dr Johann Gasteiger
Computer-Chemie-Centrum
Universitaet Erlangen
91052 Erlangen, GERMANY

Professor Michael Gribskov
San Diego Supercomputer Center
P.O. Box 85608, San Diego
CA 92186-9784, U.S.A.

Professor Peter A. Kollman
Department of Pharmaceutical Chemistry
University of California, San Francisco
CA 94143, U.S.A.

Dr A. K. Konopka
BioLingua Research
10143 Ridgeline Drive, Gaithersburg,
MD 20879, U.S.A.

Professor James A. McCammon
Department of Chemistry & Biochemistry
University of California at San Diego
La Jolla, CA 92093-0365, U.S.A.

Professor Afonso Nino
E.U. Informatica de Ciudad Real
Universidad de Castilla-la Mancha
Ronda de Calatrava No. 5
13071 Ciudade Real, SPAIN

Professor Iwao Ohmine
Chemistry Department,
Faculty of Science, Nagoya University,
Furo-cho, Chikusa, Nagoya, JAPAN

Dr Arthur Olson
Research Institute of the Scripps Clinic
10666 North Torrey Pines Road
La Jolla, CA 92037, U.S.A.

Professor Isaiah Shavitt
Department of Chemistry
Ohio State University, Columbus
OH 43210, U.S.A.

Professor T. Shida
Department of Chemistry
Faculty of Sciences, Kyoto University
Kyoto 606, JAPAN

Professor Andrzej Sokalski
Molecular Modelling Laboratory
Technical University of Wroclaw
Wyb. Wyspianskiego 27
50-370 Wroclaw, POLAND

Dr W. R. Taylor
Laboratory for Mathematical Biology
National Institute for Medical Research
The Ridgeway, Mill Hill
London NW7 1AA, ENGLAND

Professor Nenad Trinajstic
Institut Rugjer Boskovic
P.O. Box 1016, 41001 Zagreb
CROATIA

Professor Charles L. Wilkins
Department of Chemistry
University of California, Riverside
CA 92521, U.S.A.

Publishing and Advertising Offices

Elsevier Science Ireland Ltd., Bay 15k, Shannon Ind. Estate, Shannon, Co. Clare, Ireland. Tel.: (+353) 61 471944, Fax: (+353) 61 472144. Authors wishing to use e-mail to contact the Elsevier Science Production Editor for *Computers and Chemistry* may use the following address: chemistry.production@elsevier.co.uk. It is recommended that the journal name is put in the subject field of the message's "envelope" information.

Frequency: Published every two months in January, March, May, July, September and November

Subscription Information

Annual Institutional Subscription Rates 1998: Europe, The CIS and Japan 1852 Dutch Guilders. All other countries U.S.$1064. Dutch Guilder prices exclude VAT. Non-VAT registered customers in the European Community will be charged the appropriate VAT in addition to the price listed. Prices include postage and insurance and are subject to change without notice. Any enquiry relating to subscriptions should be sent to: **The Americas**: Elsevier Science Customer Support Department, P.O. Box 945, New York, NY 10010, U.S.A. [Tel: (+1) 212-633-3730/1-888 4ES-INFO. Fax: (+1) 212-633-3680. E-mail: usinfo-f@elsevier.com]. **Japan**: Elsevier Science Customer Support Department, 9-15 Higashi-Azabu 1-chome, Minato-ku, Tokyo 106-0044, Japan [Tel: (+3) 5561-5033. Fax: (+3) 5561-5047. E-mail: info@elsevier.co.jp]. **Asia Pacific (*excluding Japan*)**: Elsevier Science (Singapore) Pte Ltd, No. 1 Temasek Avenue, 17-01 Millennia Tower, Singapore 039192 [Tel: (+65) 434-3727. Fax: (+65) 337-2230. E-mail: asiainfo@elsevier.com.sg]. **Rest of the World**: Elsevier Science Customer Service Department, P.O. Box 211, 1001 AE Amsterdam, The Netherlands [Tel: (+31) 20-485-3757. Fax: (+31) 20-485-3432. E-mail: nlinfo-f@elsevier.nl].

Copyright © 1998 Elsevier Science Ltd

PERIODICALS POSTAGE PAID AT RAHWAY, NEW JERSEY. *Computers and Chemistry* (ISSN 0097-8485) is published 6 issues per year in January, March, May, July, September and November by Elsevier Science Ltd, The Boulevard, Langford Lane, Kidlington, Oxford OX5 1GB, U.K. The annual subscription in the U.S.A. is $876. *Computers and Chemistry* is distributed by Mercury Airfreight International Ltd, 10 Camptown Road, Irvington, NJ 07111-1105. POSTMASTER: Please send address corrections to *Computers and Chemistry*, c/o Elsevier Science Inc., RSO, Customer Support Department, 655 Avenue of the Americas, New York, NY 10010, U.S.A. [Tel.: (+1) 212-633-3730/1 888 4ES-INFO. Fax: (+1) 212-633-3680. E-mail: usinfo-f@elsevier.com].

List of Contents

NUMBER 1

FOURTH CONFERENCE ON COMPUTERS IN CHEMISTRY AND THE THIRD CONFERENCE ON COMPUTER-AIDED RESEARCH IN SCIENCE AND TECHNOLOGY

Foreword
W. A. Sokalski and H. Chojnacki 1 Fourth Conference on Computers in Chemistry and the Third Conference on Computer-Aided Research in Science and Technology

SECTION 1: COMPUTATIONAL QUANTUM CHEMISTRY

S. Roszak and H. Chojnacki 3 The Performance of the Density Functional Theory on Reaction Pathways Requiring the Multideterminant Description

K. Strasburger 7 Approximate Representation of the Molecular Electron Density. An Application to the Water Dimer and Solvated Positron

A. Jaworski 13 Application of Reaction Path Concept in Intramolecular Proton Transfer

SECTION 2: MOLECULAR SIMULATIONS OF LARGE MOLECULAR AGGREGATES

W. M. Gańcza and T. Paszkiewicz 21 The Application of Object-oriented Programming to Monte Carlo Experiments on Beams of Phonons in Crystals

W. Bartkowiak and J. Lipiński 31 Solvent Effect on the Nonlinear Optical Properties of Para-nitroaniline Studied by Langevin Dipoles–Monte Carlo (LD/MC) Approach

H. Galina and J. Lechowicz 39 An Algorithm for Monte Carlo Modeling of Degradation of Polymer Networks

E. Hawlicka and D. Swiatla-Wojcik 43 MD Simulation of a NaCl solution in Equimolar Methanol–water Mixture

W. Nowak 49 Computer Modelling of Dynamics of Ser92X Deoxymyoglobin Mutants

I. Roterman, J. Rybarska, L. Konieczny, M. Skowronek, B. Stopa, B. Piekarska and G. Bakalarski 61 Congo Red Bound to α-1-proteinase Inhibitor as a Model of Supramolecular Ligand and Protein Complex

W. M. Bartczak, K. Wolf and A. Hummel 71 Computer Simulation Studies of Recombination of Ions in Multi Ion-pair Ensembles I. Diffusion-controlled Processes

W. M. Bartczak and A. Hummel 79 Computer Simulation Studies of Recombination of Ions in Multi Ion-pair Ensembles II. Processes Characterized by Long Mean Free Paths of Charged Species

SECTION 3: EXPERIMENTAL DATA PROCESSING

K. T. Wojciechowski, A. Malecki and B. Prochowska-Klisch 89 REACTKIN—a Program for Modelling the Chemical Reactions in Electrolytes Solutions

J. P. Hawranek and A. S. Muszyński 95 On the Determination of Optical Constants of Liquids in the Infrared Region

W. Wrzeszcz, A. S. Muszyński and J. P. Hawranek 101 Analysis of IR Thin-film Transmission Spectra of Liquid Tri-*n*-*propylamine*

S. Tryka 113 Cut-off Filter Method for Light-induced Photon Emission Spectra Estimation

W. B. Mroczyk and K. M. Michalski 119 Application of Modern Computer Methods for Recognition of Chemical Compounds in NIRS

J. Leluk 123 A New Algorithm for Analysis of the Homology in Protein Primary Structure

SECTION 4: KNOWLEDGE ENGINEERING

Z. S. Hippe 133 Design and Application of an Intelligent Information System SCANKEE® for Solving Selected Chemical Problems

G. Fic and G. Nowak 141 Extended Concept of Reaction Generators in an Organic Reaction Prediction System CSB

G. Nowak and G. Fic 147 Implementation of Commonsense Reasoning in Organic Reaction Prediction System CSB

B. J. Dębska 153 Knowledge Transform from a Set of Cases to Production Rule Knowledgebase

Announcement I

NUMBERS 2/3

César L. Araujo, Gabriela A. Ibañez, Gabriela N. Ledesma, Graciela M. Escandar and Alejandro C. Olivieri 161 EPSILON: a Versatile Microcomputer Program for the Spectrophotometric Data Analysis of Metal–Ligand Equilibria

John M. Herbert and **Walter C. Ermler** 169 Symbolic Implementation of Arbitrary-order Perturbation Theory using Computer Algebra: Application to Vibrational–Rotational Analysis of Diatomic Molecules

T. E. Simos and **P. S. Williams** 185 Computer Algebra Programmes for the Construction of a Family of Numerov-type Exponentially-fitted Methods for the Numerical Solution of the Schrödinger equation

E. Mischler, F. Humbert and **D. Canet** 219 NMR Pulse Sequence Generator for a PC Driven Spectrometer

Juan F. Van der Maelen Uría and **Carmen Alvarez-Rúa Alvarez** 225 Using Spline Functions for Obtaining Accurate Partial Molar Volumes in Binary Mixtures

D. Britz 237 Time shift artifacts and start-up protocols with the BDF method in electrochemical digital simulation

Reuben Rudman 245 Geometric Enclosures: a New Notation for Chemical Symbols

Christopher Coomber 251 Current Theories of Neuronal Information Processing Performed by Ca^{2+}/Calmodulin-dependent Protein Kinase II with Support and Insights from Computer Modelling and Simulation

Book Review
Jonathan Bowen 265 Modern Compiler Implementation in C: Basic Techniques, Modern Compiler Implementation in Java: Basic Techniques, Modern Compiler Implementation in ML: Basic Techniques, by Andrew W. Appel

NUMBER 4

I. Strokov 269 One more macropackage for typesetting structural formulae with LaTeX

D. Juretić, D. Zucić, B. Lučić and **N. Trinajstić** 279 Preference functions for prediction of membrane-buried helices in integral membrane proteins

J. C. Phillips 295 Algebraic constructs for the graphical and computational solution to balancing chemical equations

T.-H. Lin, W.-J. Peng and **Y.-J. Lu** 309 Identification of convexity as a common structure feature for structures generated for two short peptides

A. D. Maine and **P. Xia** 321 High-speed manipulation of information representations. I. Normalization and mobile canonicalization

W. J. Pullan 331 Genetic operators for a two-dimensional bonded molecular model

A. I. Denesyuk, K. A. Denessiouk, V. P. Zav'Yalov, J. Lundell and **T. Korpela** 339 Analogous conformations of both binding and effector regions in cyclosporin A, FK506 and rapamycin

M. Keser and **S. I. Stupp** 345 A genetic algorithm for conformational search of organic molecules: implications for materials chemistry

Book Review
T. E. Simos 353 "An introduction to computational physics" by Tao Pang

NUMBER 5

Camelia Muñoz-Caro and **Alfonso Niño** 355 Neural modeling of torsional potential hypersurfaces in non-rigid molecules

K. Wieczorek-Ciurowa 363 Application of optimization methods to solid phase analysis of combustion gases desulphurization products

M. J. L. Schoonman, R. M. A. Knegtel and **P. D. J. Grootenhuis** 369 Practical evaluation of comparative modelling and threading methods

M. M. Pariona and **I. L. Müller** 377 Numerical simulation and factorial design of titanium crevice corrosion in sodium chloride solution

Zhao Weixiang, Chen Dezhao and **Hu Shangxu** 385 Potential function based neural networks and its application to the classification of complex chemical patterns

Xu Lu and **Jia-An Yang** 393 Chemical environment code and measure of molecular similarity

Paulo Fernando Bruno Gonçalves, Mariane Axt, Valentim Emílio Uberti Costa and **Paolo Roberto Livotto** 399 Determination of NMR shift reagent position by the pseudocontact model

Aixia Yan, Ruisheng Zhang, Mancang Liu, Zhide Hu, M. A. Hooper and **Zhengfeng Zhao** 405 Large artificial neural networks applied to the prediction of retention indices of acyclic and cyclic alkanes, alkenes, alcohols, esters, ketones and ethers

G. Huybrechts and **G. Van Assche** 413 Software Note
OPTKIN-Mechanistic modeling by kinetic and thermodynamic parameter optimization

Lee F. Brown and **Michael H. Ebinger** 419 Modeling precipitation from concentrated solutions with the EQ3/6 chemical speciation codes

G. L. Aranovich and **M. D. Donohue** 429 A simple numerical algorithm for solution of non-linear equations with multiple roots

T. E. Simos 433 New embedded explicit methods with minimal phase-lag for the numerical integration of the Schrödinger equation

Book Reviews

J. Varley 441 Computational transport phenomena: Numerical methods for the solution of transport problems

J. Crabbe 443 Excel for chemists

NUMBER 6

S. Olszewski and **T. Kwiatkowski** 445 A topological approach to evaluation of non-degenerate Schrödinger perturbation energy based on a circular scale of time

Michel Petitjean 463 Interactive maximal common 3D substructure searching with the combined SDM/RMS algorithm

T. E. Simos 467 An eighth order exponentially-fitted method for the numerical integration of the Schrödinger equation

Michael D. Thomas and **Gordon L. Hug** 491 A computer-controlled nanosecond laser system

Andrzej J. Goraczko 499 Simplification of mass spectra of organometallic and coordination compounds by cluster profile analysis

Ján Mikuláš Lisý and **Peter Šimon** 509 Evaluation of parameters in nonlinear models by the least squares method

Saikia Arupjyoti and **Suryanarayana Iragavarapu** 515 New electrotopological descriptor for prediction of boiling points of alkanes and aliphatic alcohols through artificial neural network and multiple linear regression analysis

P. A. D. de Maine 523 High-speed manipulation of information representations. II. Markush (fragment) searches

Book Review

James Crabbe 539 Biological sequence analysis: probabilistic models of proteins and nucleic acids

AUTHOR INDEX

Alvarez-Rúa Alvarez C., 225
Aranovich G. L., 429
Araujo C. L., 161
Arupjyoti S., 515
Axt M., 399

Bakalarski G., 61
Bartczak W. M., 71, 79
Bartkowiak W., 31
Bowen J., 265
Britz D., 237
Brown L. F., 419
Bruno Gonçalves P. F., 399

Canet D., 219
Chojnacki H., 1, 3
Coomber C., 251
Crabbe J., 443, 539

Dębska B. J., 153
Denessiouk K. A., 339
Denesyuk A. I., 339
Dezhao C., 385
Donohue M. D., 429

Ebinger M. H., 419
Ermler W. C., 169
Escandar G. M., 161

Fic G., 141, 147

Galina H., 39
Gańcza W. M., 21
Goraczko A. J., 499
Grootenhuis P. D. J., 369

Hawlicka E., 43
Hawranek J. P., 95, 101
Herbert J. M., 169
Hippe Z. S., 133
Hooper M. A., 405
Hu Z., 405
Hug G. L., 491
Humbert F., 219
Hummel A., 71, 79
Huybrechts G., 413

Ibañez G. A., 161
Iragavarapu S., 515

Jaworski A., 13
Juretić D., 279

Keser M., 345
Knegtel R. M. A., 369
Konieczny L., 61
Korpela T., 339
Kwiatkowski T., 445

Lechowicz J., 39
Ledesma G. N., 161
Leluk J., 123
Lin T.-H., 309
Lipiński J., 31
Lisý J. M., 509
Liu M., 405
Livotto P. R., 399
Lu X., 393
Lu Y.-J., 309
Lučić B., 279
Lundell J., 339

Maine A. D., 321
de Maine P. A. D., 523
Malecki A., 89
Michalski K. M., 119
Mischler E., 219
Mroczyk W. B., 119
Müller I. L., 377
Muñoz-Caro C., 355
Muszyński A. S., 95, 101

Niño A., 355
Nowak G., 141, 147
Nowak W., 49

Olivieri A. C., 161
Olszewski S., 445

Pariona M. M., 377
Paszkiewicz T., 21
Peng W.-J., 309
Petitjean M., 463
Phillips J. C., 295

Piekarska B., 61
Prochowska-Klisch B., 89
Pullan W. J., 331

Roszak S., 3
Roterman I., 61
Rudman R., 245
Rybarska J., 61

Schoonman M. J. L., 369
Shangxu H., 385
Šimon P., 509
Simos T. E., 185, 353, 433, 467
Sk[illegible]ronek M., 61
S[illegible]lski W. A., 1
Stępa B., 61
Strasburger K., 7
Strokov I., 269
Stupp S. I., 345
Swiatla-Wojcik D., 43

Thomas M. D., 491
Trinajstić N., 279
Tryka S., 113

Uberti Costa V. E., 399

Van Assche G., 413
Van der Maelen Uría J. F., 225
Varley J., 441

Weixiang Z., 385
Wieczorek-Ciurowa K., 363
Williams P. S., 185
Wojciechowski K. T., 89
Wolf K., 71
Wrzeszcz W., 101

Xia P., 321

Yan A., 405
Yang J-A., 393

Zav'Yalov V. P., 339
Zhang R., 405
Zhao Z., 405
Zucić D., 279

Typeset in Great Britain by BPC Digital Techset Ltd, Exeter. Printed by BPC Wheatons Ltd, Exeter